

How does degree heterogeneity affect nucleation of Ising model on complex networks?

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We investigate the nucleation of Ising model on complex networks and focus on the role played by the heterogeneity of degree distribution on nucleation rate. Using Monte Carlo simulation combined with forward flux sampling, we find that for a weak external field the nucleation rate decreases monotonically as degree heterogeneity increases. Interestingly, for a relatively strong external field the nucleation rate exhibits a nonmonotonic dependence on degree heterogeneity, in which there exists a maximal nucleation rate at an intermediate level of degree heterogeneity. Furthermore, we develop a heterogeneous mean-field theory for evaluating the free-energy barrier of nucleation. The theoretical estimations are qualitatively consistent with the simulation results. Our study suggests that degree heterogeneity plays a nontrivial role in the dynamics of phase transition in networked Ising systems.

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I. INTRODUCTION

Since many social, biological, and physical systems can be properly described by complex networks, dynamics on complex networks have received considerable attention in recent decades [1–4]. In particular, phase transitions on complex networks have been a subject of intense research in the field of statistical physics and many other disciplines [5]. Owing to the heterogeneity in degree distribution, phase transitions on complex networks are drastically different from those on regular lattices in Euclidean space. For instance, degree heterogeneity can lead to a vanishing percolation threshold [6], the whole infection of disease with any small spreading rate [7], the Ising model to be ordered at all temperatures [8–10], the transition from order to disorder in voter models [11], synchronization to be suppressed [12, 13] and different path towards synchronization in oscillator network [14], just to list a few. However, there is much less attention paid to the dynamics of phase transition itself on complex networks, such as nucleation process in a first-order phase transition.

Nucleation is a fluctuation-driven process that initiates the decay of a metastable state into a more stable one [15]. Many important phenomena in nature, like crystallization [16], glass formation [17], and protein folding [18] are closely related to nucleation process. In the context of complex networks, the study of nucleation process is not only of theoretical importance for understanding how a first-order phase transition happens in networked systems, but also may have potential implications in real situations, such as the transitions between different dy-

namical attractors in neural networks [19] and the genetic switch between high and low-expression states in gene regulatory networks [20, 21], and opinion revolution [22] as well as language replacement [23, 24] in social networks.

Recently, we have made the first step for studying nucleation process of Ising model on complex networks, where we have identified that nucleation pathways using rare-event sampling technique, such as nucleating from nodes with smaller degree on heterogeneous networks [25] and multi-step nucleation process on modular networks [26]. In addition, we found that the size-effect of the nucleation rate on mean-field-type networks [25] and non-monotonic dependence of the nucleation rate on modularity of networks [26]. As mentioned above, degree heterogeneity has a significant effect on dynamics on complex networks. Therefore, a natural question arises: how degree heterogeneity affects nucleation of Ising model on complex networks? To answer this question, in this paper, we study the dynamics of nucleation on various network models whose heterogeneity of degree distribution can be continuously changed by adjusting a single parameter. We use Monte Carlo (MC) simulation combined with forward flux sampling (FFS) to compute the nucleation rate and consider the effect of degree heterogeneity on the rate. Since the critical temperature of Ising model on uncorrelated random networks increases with the heterogeneity of degree distribution [5, 8–10], one may come to an intuitive conclusion: if both the temperature and external field are fixed, the nucleation rate will decrease monotonically as degree heterogeneity increases. Here, we show that such an intuition is not the case: the nucleation rate can change monotonically or nonmonotonically with degree heterogeneity depending on the level of driving force, i.e., the value of external field. For a weak external field, the nucleation rate decreases monotonically

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with degree heterogeneity, whereas for a relatively strong external field there exists a maximal nucleation rate corresponding to a moderate level of degree heterogeneity. Furthermore, we present a heterogeneous mean-field theory for calculating free-energy barrier of nucleation. The theoretical results qualitatively agree with the simulation ones.

II. MODEL AND SIMULATION DESCRIPTIONS

The Ising model in a network comprised of N nodes is described by the Hamiltonian

$$\mathcal{H} = -J \sum_{i < j} a_{ij} s_i s_j - h \sum_i s_i, \quad (1)$$

where spin variable s_i at node i takes either +1 (up) or -1 (down). $J(>0)$ is the coupling constant and h is the external field imposed on each node. The elements of the adjacency matrix of the network take $a_{ij} = 1$ if nodes i and j are connected and $a_{ij} = 0$ otherwise.

The simulation is performed by standard Metropolis spin-flip dynamics, in which we attempt to flip each spin once, on average, during each MC cycle. In each attempt, a randomly chosen spin is flipped with the probability $\min(1, e^{-\beta \Delta E})$, where $\beta = 1/(k_B T)$ with the Boltzmann constant k_B and the temperature T , and ΔE is the energy change due to the flipping process. We set $h > 0$ and $T < T_c$, where T_c is the critical temperature. The initial configuration is prepared with a metastable state in which $s_i = -1$ for most of the spins. The system will stay in that state for a significantly long time before undergoing a nucleating transition to the thermodynamic stable state with most spins pointing up.

Since nucleation is an activated process that occurs extremely slow, brute-force simulation is prohibitively expensive. To overcome this difficulty, we will use a recently developed simulation method, FFS [27]. This method allows us to calculate nucleation rate and determine the properties of ensemble toward nucleation pathways. The simulation results below are obtained by averaging over at least 5 independent FFS samplings and 10 different network realizations.

III. RESULTS

To study the effect of degree heterogeneity on nucleation, we first adopt a network model proposed in Ref.[28]. The network model allows us to construct networks with the same mean degree, interpolating from Erdo-Reñyi (ER) graphs to Barabaši-Albert (BA) SF networks by tuning a single parameter δ_{ERBA} . For $\delta_{ERBA} = 0$ one gets ER graphs with a Poissonian degree distribution whereas for $\delta_{ERBA} = 1$ the resulting networks are SF with $P(k) \sim k^{-3}$. Increasing δ_{ERBA}

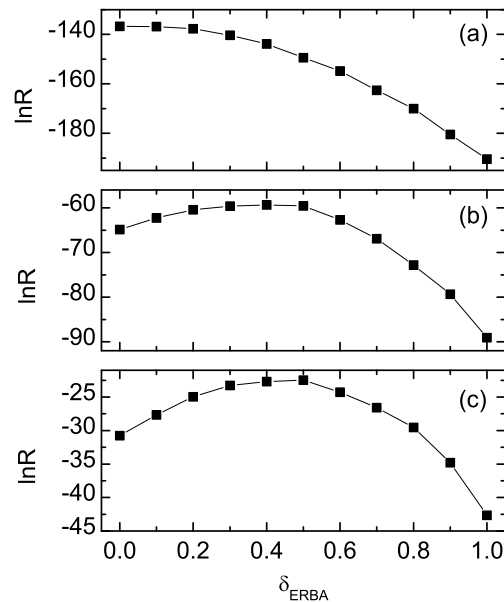


FIG. 1: The logarithm of the nucleation rate $\ln R$ as a function of the strength of degree heterogeneity δ_{ERBA} for $h = 0.5$ (a), $h = 0.8$ (b), and $h = 1.0$ (c). Other parameters are $N = 1000$, the mean degree $\langle k \rangle = 6$, and $T = 2.5$.

from 0 to 1, the degree heterogeneity of the network increases. Fig.1 shows that the logarithm of the nucleation rate $\ln R$ as a function of δ for three different external fields: $h = 0.5$, 0.8 , and 1.0 . For $h = 0.5$, $\ln R$ decreases monotonically with δ_{ERBA} , implying that degree heterogeneity is unfavorable for the occurrence of nucleation events. Interestingly, for $h = 0.8$ $\ln R$ is no longer monotonically dependent on δ_{ERBA} : as degree heterogeneity increases, $\ln R$ first increases slowly until $\delta_{ERBA} = 0.5$ and then decreases rapidly. Further increasing h to $h = 1.0$, $\ln R$ clearly exhibits a nonmonotonic change with δ_{ERBA} . That is, there exists a maximal nucleation rate that occurs at a moderate strength of degree heterogeneity.

To understand the above simulation results, we shall give a heterogeneous mean-field theory on complex networks for evaluating the nucleation barrier. First, we define m_k as the average magnetization of a node with degree k , i.e., $m_k = N_k^{-1} \sum_{i|k_i=k} s_i$, where N_k is the number of nodes with degree k . Furthermore, for a network without degree correlation, the probability that a randomly chosen nearest neighbor node has degree k is $kP(k)/\langle k \rangle$, where $P(k) = N_k/N$ is degree distribution and $\langle k \rangle = \sum_k kP(k)$ is the mean degree. Thus, the interaction energy between a node with degree k and its neighboring nodes can be expressed as $-J k m_k \sum_{k'} k' P(k') m_{k'} / \langle k \rangle$. The total energy of the net-

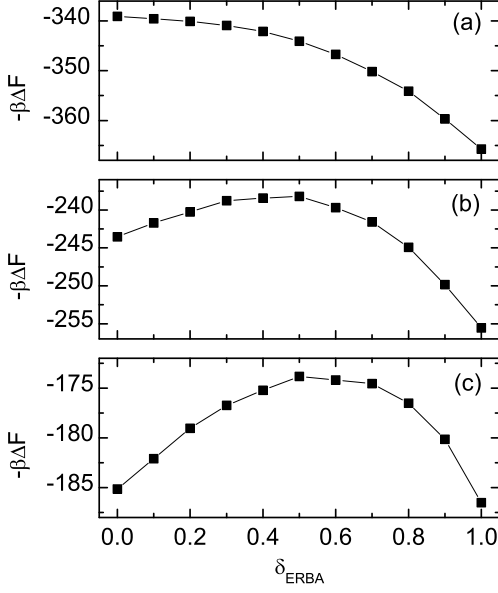


FIG. 2: Theoretical results of $-\beta\Delta F$ as a function of δ_{ERBA} for $h = 0.5$ (a), $h = 0.8$ (b), and $h = 1.0$ (c). Other parameters are the same as those in Fig.1.

work can be written as

$$\begin{aligned} E &= -\frac{1}{2}J \sum_k N_k k m_k \sum_{k'} \frac{k' P(k') m_{k'}}{\langle k \rangle} - h \sum_k N_k m_k \\ &= -\frac{1}{2}N J \langle k \rangle m'^2 - N h m, \end{aligned} \quad (2)$$

where

$$m' = \sum_k \frac{k P(k) m_k}{\langle k \rangle} \quad (3)$$

is the average magnetization of a randomly chosen nearest neighbor node, and $m = \sum_k P(k) m_k$ is the average magnetization of a randomly chosen node. Note that m' differs from m in general. Special cases for which $m' = m$ are provided by k -independent quantities $m_k = m$. In particular, for the all-spin down configuration with $m_k = -1$ for all k and for the all-spin-up configuration with $m_k = 1$ for all k , one has $m' = m = -1$ and $m' = m = 1$, respectively.

Defining S_k as the entropy of a node with degree k , the total entropy of the network is

$$S = \sum_k N_k S_k = N \sum_k P(k) S_k, \quad (4)$$

with

$$S_k = -k_B \left[\frac{1+m_k}{2} \ln \left(\frac{1+m_k}{2} \right) + \frac{1-m_k}{2} \ln \left(\frac{1-m_k}{2} \right) \right]. \quad (5)$$

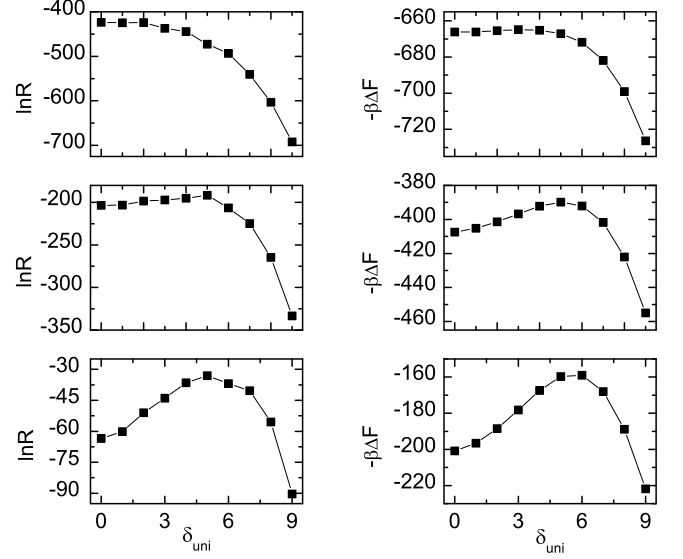


FIG. 3: Simulation (left panels) and theoretical (right panels) results on networks with uniform degree distribution. The external fields from top to bottom are $h = 1.0$, 2.0 , and 3.0 , respectively. Other parameters are $N = 1000$, the mean degree $\langle k \rangle = 10$, and $T = 3$.

Combining Eq.2 and Eq.4, we can get the expression of free energy, i.e., $F = E - TS$.

At the minimum and maximum points of free energy, we have $\partial F / \partial m_k = 0$, which yields the mean-field equation of m_k [5, 9],

$$m_k = \tanh [\beta h + \beta J k m']. \quad (6)$$

Substituting Eq.6 into Eq.3, we get

$$m' = \sum_k \frac{k P(k)}{\langle k \rangle} \tanh [\beta h + \beta J k m']. \quad (7)$$

Eq.7 is a self-consistent equation of m' that can be numerically solved. In the present settings, Eq.7 has three solutions: m'_- , m'_0 , and m'_+ , where m'_\pm are stable solutions and m'_0 is unstable one. Inserting the three solutions of m' into the rsh of Eq.6, we can obtain m_k , and then get E_α , S_α and F_α ($\alpha = -, 0, +$) according to Eq.2 and Eq.4. Since $h > 0$, we have $F_0 > F_- > F_+$, which gives the free-energy barrier from metastable to stable state $\Delta F = F_0 - F_-$ and thus estimate the nucleation rate $R \sim \exp(-\beta\Delta F)$.

Theoretical results of $-\beta\Delta F$ as a function of δ are shown in Fig.2, where the parameters are the same as those in Fig.1. It is clear that the theoretical results are qualitatively consistent with the simulation ones.

In order to check the generality of the above results, we shall calculate nucleation rate on some other network models by both numerical simulations and theory.

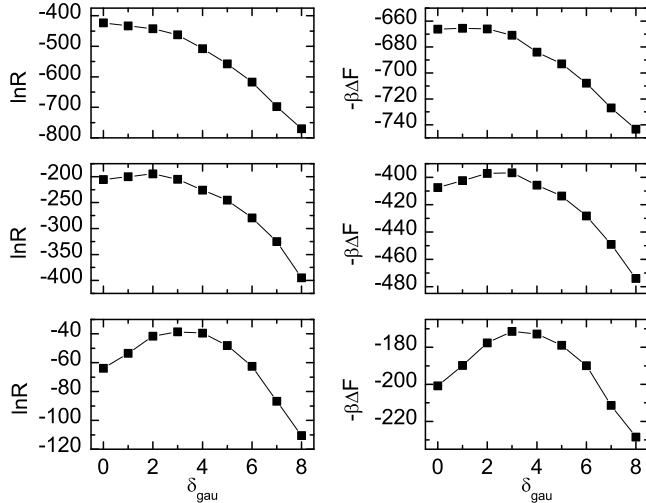


FIG. 4: Simulation (left panels) and theoretical (right panels) results on networks with Gaussian degree distribution. The external fields from top to bottom are $h = 1.0, 2.0$, and 3.0 , respectively. Other parameters are $N = 1000$, the mean degree $\langle k \rangle = 10$, and $T = 3$.

Firstly, we construct a network with uniform degree distribution in which node degree is randomly selected in the range $[\langle k \rangle - \delta_{uni}, \langle k \rangle + \delta_{uni}]$, where δ_{uni} is an integer between 0 and $\langle k \rangle - 1$ that controls the strength of degree heterogeneity. The network is generated according to the Molloy-Reed algorithm [29]. This construction eliminates the degree correlations between neighboring nodes. Fig.3 shows the simulation and theoretical results, from which the similar phenomena are also present: for weak external field the nucleation rate decreases monotonically with degree heterogeneity, while for strong external field the

nucleation rate varies nonmonotonically with degree heterogeneity. Moreover, we construct a network with Gaussian degree distribution with fixed mean degree $\langle k \rangle$ and variance δ_{gau} . As shown in Fig.4, both the simulation and theoretical results display the similar phenomena.

IV. SUMMARY

In summary, using Ising model on complex networks we have shown how degree heterogeneity affects the rate of nucleation. The main results of the present paper are that for a weak external field the nucleation rate decreases monotonically as degree heterogeneity increases, whereas for a relatively strong external field the nucleation rate first increases and then decreases with the increment of degree heterogeneity. Therefore, the nucleation rate can change monotonically or nonmonotonically with degree heterogeneity depending on the value of the external field. The results are robust to different network models, thereby verifying the generality of the results. Moreover, we have developed the so-called heterogeneous mean-field theory for calculating the free-energy barrier to nucleate and thus estimating the nucleation rate. The theory is effective in qualitatively predicting the simulation results. Our findings indicate that degree heterogeneity plays a nontrivial role in the nucleation events of Ising model on complex networks.

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- [1] R. Albert and A.-L. Barabási, *Rev. Mod. Phys.* **74**, 47 (2002).
 - [2] M. E. J. Newman, *SIAM Review* **45**, 167 (2003).
 - [3] S. Boccaletti, V. Latora, Y. Moreno, M. Chavez, and D.-U. Hwang, *Phys. Rep.* **424**, 175 (2006).
 - [4] A. Arenas, A. Díaz-Guilera, J. Kurths, Y. Moreno, and C. Zhou, *Phys. Rep.* **469**, 93 (2008).
 - [5] S. N. Dorogovtsev, A. V. Goltsev, and J. F. F. Mendes, *Rev. Mod. Phys.* **80**, 1275 (2008).
 - [6] R. Cohen, K. Erez, D. ben Avraham, and S. Havlin, *Phys. Rev. Lett.* **85**, 4626 (2000).
 - [7] R. Pastor-Satorras and A. Vespignani, *Phys. Rev. Lett.* **86**, 3200 (2001).
 - [8] A. Aleksiejuk, J. A. Holysta, and D. Stauffer, *Physica A* **310**, 260 (2002).
 - [9] G. Bianconi, *Phys. Lett. A* **303**, 166 (2002).
 - [10] S. N. Dorogovtsev, A. V. Goltsev, and J. F. F. Mendes, *Phys. Rev. E* **66**, 016104 (2002).
 - [11] R. Lambiotte, *Europhys. Lett* **78**, 68002 (2007).
 - [12] T. Nishikawa, A. E. Motter, Y.-C. Lai, and F. C. Hoppensteadt, *Phys. Rev. Lett.* **91**, 014101 (2003).
 - [13] A. E. Motter, C. Zhou, and J. Kurths, *Phys. Rev. E* **71**, 016116 (2005).
 - [14] J. Gómez-Gardeñes, Y. Moreno, and A. Arenas, *Phys. Rev. Lett.* **98**, 034101 (2007).
 - [15] D. Kashchiev, *Nucleation: basic theory with applications* (Butterworths-Heinemann, Oxford, 2000).
 - [16] S. Auer and D. Frenkel, *Nature* **409**, 1020 (2001).
 - [17] G. Johnson, A. I. Mel'cuk, H. Gould, W. Klein, and R. D. Mountain, *Phys. Rev. E* **57**, 5707 (1998).
 - [18] A. R. Fersht, *Proc. Natl. Acad. Sci. USA* **92**, 10869 (1995).
 - [19] Y. Bar-Yam and I. R. Epstein, *Proc. Natl. Acad. Sci. USA* **101**, 4341 (2004).
 - [20] T. Tian and K. Burrage, *Proc. Natl. Acad. Sci. USA* **103**, 8372 (2006).

- [21] A. Koseska, A. Zaikin, J. Kurths, and J. García-Ojalvo, PLoS ONE **4**, e4872 (2009).
- [22] R. Lambiotte and M. Ausloos, J. Stat. Mech. p. P08026 (2007).
- [23] J. Ke, T. Gong, and W. S.-Y. Wang, Commun. Comput. Phys. **3**, 935 (2008).
- [24] S. Wichmann, D. Stauffer, C. Schulze, and E. W. Holman, Adv. Complex Syst. **11**, 357 (2008).
- [25] H. Chen, C. Shen, Z. Hou, and H. Xin, Phys. Rev. E **83**, 031110 (2011).
- [26] H. Chen and Z. Hou, Phys. Rev. E **83**, 046124 (2011).
- [27] R. J. Allen, P. B. Warren, and P. R. ten Wolde, Phys. Rev. Lett. **94**, 018104 (2005).
- [28] J. Gómez-Gardeñes and Y. Moreno, Phys. Rev. E **73**, 056124 (2006).
- [29] M. Molloy and B. Reed, Random Struct. Algorithms **6**, 161 (1995).